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LLNL-TR-408568

OBES "One Pager"

J. G. Tobin

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Laboratory Name: Lawrence Livermore National Lab**B&R Code: KC 0203010****FWP/subtask Title under FWP:** Investigations of Electron Correlation in Complex Systems**FWP Number:** SCW0289**Principal Investigators:** Jim Tobin (Lead), Brandon Chung, Sung Woo Yu, G. Dan Waddill (MST)**Program Scope:** We are developing and utilizing photon dichroic and spin resolved techniques to investigate electron correlation in complex systems. These materials include potential spintronic device sources such as Fe/GaAs and f electronic materials such as non-magnetic δ -Pu.**Major Program Achievements:**

After an extensive review of our project, our funding has been increased to \$600K per year for FY09 and the program is being converted into a Multi-PI Project. B. Chung, S.W. Yu and G.D. Waddill are the new Co-PIs, joining J.G. Tobin. The Fano/BIS Spectrometer is being commissioned in B235 at LLNL. A collaboration with Dr. T. Gouder of ITU is being pursued. We have developed an alternative model for electron correlation in Pu and are pursuing its experimental benchmarking.

Refereed Journal Publications in calendar year 2008 (also 2 more Conference Proceedings):

1. J.G. Tobin, P. Söderlind, A. Landa, K.T. Moore, A.J. Schwartz, B.W. Chung, M.A. Wall, J.M. Wills, R.G. Haire, and A.L. Kutepov, "On the electronic configuration in Pu: Spectroscopy and Theory," J. Phys. Cond. Matter **20**, 125204 (2008).
2. S.W. Yu and J. G. Tobin, "Breakdown of spatial inversion symmetry in core level photoemission, Phys. Rev. B **77**, 193409 (2008).
3. J.D.W. Thompson, J.R. Neal, T.H. Shen, S.A. Morton, J.G. Tobin, G.D. Waddill, J.A.D. Matthew, D. Greig, and M. Hopkinson, "Evolution of Ga and As core levels in the formation of Fe/GaAs(001): A high-resolution soft x-ray photoelectron spectroscopic study," J. Appl. Phys. **104**, 024516 (2008).
4. S.W. Yu, J.G. Tobin, P. Söderlind, , "An alternative model for electron correlation in Pu," J. Phys. Cond. Matter **20**, 422202 (2008), Fast Track Communication.
5. J.G. Tobin, S.W. Yu, B.W. Chung and G.D. Waddill, "Resolving the Pu Electronic Structure Enigma: Past Lessons and Future Directions," J. Nucl. Mat., accepted October 2008.

Invited Talks in calendar year 2008:

1. S.W. Yu, "An alternative model for electron correlation in Pu," Actinides IV Symposium, Spring Meeting of the Materials Research Society (MRS), San Francisco, CA, USA, March 25 - 29, 2008.
2. J.G. Tobin, "An alternative model for electron correlation in Pu," Pu Futures Meeting, Dijon, France, July 8 - 11, 2008.
3. J.G. Tobin, "Observation of Dynamical Spin Shielding in Ce and Why It Matters for Pu Electronic Structure," Institute for TransUranics (ITU), Karlsruhe, Germany, July 14 - 15, 2008.
4. J.G. Tobin, "An alternative model for electron correlation in Pu," 8th International Workshop: "Fundamental Plutonium Properties" VNIITF, Snezhinsk, Chelyabinsk Reg., Russia, Sept 6 - 12, 2008.

Program Impact:

We are pursuing Double Polarization Photoelectron Dichroism measurements of the Fano Effect, using spin resolving detection in photoelectron spectroscopy, to test the nature of electron correlation in Pu. (See Pubs 2, 4 & 5.) If successful, we will solve the riddle of Pu electronic structure that has remained unresolved for the last 60 years. We are also developing a Bremsstrahlung Isochromat Spectroscopy (BIS) capability to permit the direct measurement of the unoccupied electronic structure of Pu, which is another missing piece in the puzzle of Pu electronic structure.

Interactions:

SWY was recently promoted from Postdoc to Term Employee; BWC was the lead co-chair of the Actinides IV Symposium at the 2008 Spring MRS in San Francisco, CA, USA; JGT is a lead co-chair of the upcoming Actinides 2009 International Conference in July, 2009, in San Francisco, CA, USA; JGT served on the International Advisory Committee for the Actinide XAS Meeting in Paris during July, 2008; JGT was recently elected to the MIND Executive Committee of the AVS. Collaborators - USA- National Labs: LBNL- S.A. Morton; R.G. Haire, ORNL; USA-Universities: MST-G.D. Waddill, T. Komesu; University personnel from Great Britain (See Pub 3.) Both the APS at Argonne National Laboratory and the ALS at Lawrence Berkeley National Laboratory have been used for this work. We also interact with the personnel from LANL. (See Pub 1.)

Personnel Commitments for FY2009: JG Tobin 75%, Sung Woo Yu 75%, Brandon Chung < 1%**Authorized Budget (BA) for FY06, FY07, FY08:****FY06 BA \$300,000****FY07 BA \$300,000****FY08 BA \$300,000**